Catalytic Regioselectivity Control in Ring Opening Cycloisomerization of Methylene- or Alkylidene-cyclopropyl Ketones

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Supporting Information

11h-1-158-1-cc

Archive directory: /export/home/masm/vnmrsys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
Mercury-300BB "OMC300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.500 sec
Width 19011.4 Hz
78 repetitions
OBSERVE C13, 75.4421087 MHz
DECOUPLE H1, 300.0234698 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 31 min, 48 sec

169.057

131.019

114.892

77.431
77.000
76.585

60.857

39.900
32.963
32.802
27.557
27.203
27.018
25.886
17.597
13.829

1j

1q

1u

1v

zj-23-6
Pulse Sequence: szpul

zj-23-6c

Archive directory: /export/home/ma-sm/vnmr/sys/data
Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300BB "MERCURYvx300"

0.04

Relax delay 1.000 sec

Pulse 45.0 degrees

Acq. Time 1.815 sec

Width 25000.0 Hz

10000 repetitions

OBSERVE C13, 75.4433982 MHz

DECOUPLE M1, 300.0346884 MHz

Power 35 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

FT size 131072

Total time 117 hr, 48 min, 8 sec

Mercury-300088 "MERCURYvx300"
 Relax, delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.000 sec
 Width 18867.9 Hz
 252 repetitions
 OBSERVE C13, 75.4424203 MHz
 DECOUPLE H1, 300.0310270 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 11 hr, 40 min, 7 sec

167.964
 161.102
 151.004

101.203
 98.207

60.331

32.846
 30.606
 30.350
 30.095
 29.839
 28.579
 28.324
 28.069
 27.814
 27.559
 27.304
 27.049
 26.794
 26.539
 26.284
 26.029
 25.774
 25.519
 25.264
 25.009
 24.754
 24.499
 24.244
 23.989
 23.734
 23.479
 23.224
 22.969
 22.714
 22.459
 22.204
 21.949
 21.694
 21.439
 21.184
 20.929
 20.674
 20.419
 20.164
 19.909
 19.654
 19.399
 19.144
 18.889
 18.634
 18.379
 18.124
 17.869
 17.614
 17.359
 17.104
 16.849
 16.594
 16.339
 16.084
 15.829
 15.574
 15.319
 15.064
 14.809
 14.554
 14.299
 14.044
 13.789
 13.534
 13.279
 13.024
 12.769
 12.514
 12.259
 12.004
 11.749
 11.494
 11.239
 10.984
 10.729
 10.474
 10.219
 9.964
 9.709
 9.454
 9.199
 8.944
 8.689
 8.434
 8.179
 7.924
 7.669
 7.414
 7.159
 6.904
 6.649
 6.394
 6.139
 5.884
 5.629
 5.374
 5.119
 4.864
 4.609
 4.354
 4.099
 3.844
 3.589
 3.334
 3.079
 2.824
 2.569
 2.314
 2.059
 1.804
 1.549
 1.294
 1.039
 0.784
 0.529
 0.274
 0.019

6.338
6.305

5.179
5.147

4.190
4.170
4.147
4.128

2.352
2.281
1.870
1.858
1.846
1.823
1.816
1.802
1.692
1.680
1.630
1.621
1.585
1.579
1.525
1.515
1.483
1.465
1.295
1.272
1.248

./home/zhu-hp/vnmr/sys/data

Ambient temperature
Mercury-300BB "MERCURYvx300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.500 sec
Width 18867.9 Hz
316 repetitions
OBSERVE C13, 75.4420953 MHz
DECOUPLE H1, 300.0294698 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 4 hr, 45 min, 16 sec

port/home/ma-sm/vnmr/sys/data

ictory: /export/home/masm/vnmrsys/data
 ctory:
 ce: 2pul
 C13
 perature
 86c
 B "MERCURYvx300"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.000 sec
 Width 18867.9 Hz
 62 repetitions
 OBSERVE C13, 75.4420987 MHz
 DECOUPLE H1, 300.0294698 MHz
 Power 48 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 14 hr, 55 min, 7 sec